

WHAT IS CLAIMED IS:

- 1 1. A method for predicting nucleic acid hybridization
2 thermodynamics, the method comprising:
3 providing a database of thermodynamics parameters;
4 receiving hybridization information which represents at least one
5 sequence;
6 receiving correction data;
7 receiving a first set of data which represents hybridization conditions;
8 and
9 calculating hybridization thermodynamics including net hybridization
10 thermodynamics based on the hybridization information, the thermodynamic
11 parameters, the correction data and the first set of data.
- 1 2. The method as claimed in claim 1 wherein the hybridization
2 thermodynamics of individual single stranded, bimolecular and higher order
3 complexes are statistically weighted in a numerical process and the equilibrium
4 concentration of each species is output.
- 1 3. The method as claimed in claim 2 wherein the correction data
2 includes folding correction data.
- 1 4. The method as claimed in claim 2 wherein the correction data
2 includes linear correction data.
- 1 5. The method as claimed in claim 1 wherein the thermodynamic
2 parameters include DNA thermodynamic parameters.
- 1 6. The method as claimed in claim 5 wherein the DNA
2 thermodynamic parameters include dangling end parameters.
- 1 7. The method as claimed in claim 5 wherein the DNA
2 thermodynamic parameters include coaxial stacking parameters.

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1 8. The method as claimed in claim 5 wherein the DNA
2 thermodynamic parameters include terminal mismatch parameters.

1 9. The method as claimed in claim 1 wherein the thermodynamic
2 parameters include RNA thermodynamic parameters.

1 10. The method as claimed in claim 1 wherein the thermodynamic
2 parameters include hybrid DNA/RNA thermodynamic parameters.

1 11. The method as claimed in claim 1 wherein the thermodynamic
2 parameters include DNA loop thermodynamic parameters.

1 12. The method as claimed in claim 1 wherein the hybridization
2 information represents top and bottom strand sequences which form a duplex and
3 wherein the hybridization thermodynamics are calculated for the duplex.

1 13. The method as claimed in claim 1 wherein the hybridization
2 information represents at least a section of a target and a length of at least one
3 primer or probe complimentary to the target.

1 14. The method as claimed in claim 13 wherein the hybridization
2 thermodynamics are calculated for a plurality of primers or probes complimentary
3 to the target.

1 15. The method as claimed in claim 1 wherein the hybridization
2 information represents at least a section of a target and a primer or probe.

1 16. The method as claimed in claim 15 wherein a length of the
2 target is longer than a length of the primer or probe and wherein the hybridization
3 thermodynamics are calculated for a best target/primer or target/probe complex and
4 for competitive mismatch complexes.

1 30. The system as claimed in claim 21 wherein the
2 thermodynamic parameters include hybrid DNA/RNA thermodynamic parameters.

1 31. The system as claimed in claim 21 wherein the
2 thermodynamic parameters include DNA loop thermodynamic parameters.

1 32. The system as claimed in claim 21 wherein the hybridization
2 information represents top and bottom strand sequences which form a duplex and
3 wherein the hybridization thermodynamics are calculated for the duplex.

1 33. The system as claimed in claim 21 wherein the hybridization
2 information represents at least a section of a target and a length of at least one
3 primer or probe complimentary to the target.

1 34. The system as claimed in claim 33 wherein the hybridization
2 thermodynamics are calculated for a plurality of primers or probes complimentary
3 to the target.

1 35. The system as claimed in claim 21 wherein the hybridization
2 information represents at least a section of a target and a primer or probe.

1 36. The system as claimed in claim 35 wherein a length of the
2 target is longer than a length of the primer or probe and wherein the hybridization
3 thermodynamics are calculated for a best target/primer or target/probe complex and
4 for competitive mismatch complexes.

1 37. The system as claimed in claim 34 wherein hybridization
2 information represents at least a section of a target and a primer or probe and
3 wherein a length of a target is longer than the length of the primer or probe and
4 wherein the hybridization thermodynamics are calculated for a best target/primer
5 or target/probe complex and for competitive target/primer or target/probe
6 complexes.

1 38. The system as claimed in claim 22 further comprising means
2 for calculating concentration of each species in a solution at a plurality of
3 temperatures.

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1 39. The system as claimed in claim 38 wherein hybridization
2 information also represents a primer or probe and wherein the length of the target
3 is longer than a length of the primer or probe and wherein the hybridization
4 thermodynamics are calculated for a best target/primer or target/probe complex and
5 for competitive mismatch complexes and wherein the system further comprises
6 means for calculating concentration of every species in a solution at a plurality of
7 temperatures.

1 40. The system as claimed in claim 39 wherein the hybridization
2 thermodynamics are calculated for at least two best target/primer or target/probe
3 complexes and for their corresponding competitive mismatch complexes and
4 wherein the system further comprises means for correcting for any interactions
5 between the at least two best target/primer or target/probe complexes and their
6 components.

1 41. A computer-readable storage medium having stored therein
2 a database of thermodynamics parameters and a computer program which executes
3 the steps of:
4 receiving hybridization information which represents at least one
5 sequence;
6 receiving correction data;
7 receiving a first set of data which represents hybridization conditions;
8 and
9 calculating hybridization thermodynamics including net hybridization
10 thermodynamics based on the hybridization information, the thermodynamic
11 parameters, the correction data and the first set of data.

1 42. The storage medium as claimed in claim 41 wherein the
2 hybridization thermodynamics of individual single stranded, bimolecular and higher
3 order complexes are statistically weighted in a numerical process and the
4 equilibrium concentration of each species is output.

1 43. The storage medium as claimed in claim 42 wherein the
2 correction data includes folding correction data.

1 44. The storage medium as claimed in claim 42 wherein the
2 correction data includes linear correction data.

1 45. The storage medium as claimed in claim 41 wherein the
2 thermodynamic parameters include DNA thermodynamic parameters.

1 46. The storage medium as claimed in claim 45 wherein the DNA
2 thermodynamic parameters include dangling end parameters.

1 47. The storage medium as claimed in claim 45 wherein the DNA
2 thermodynamic parameters include coaxial stacking parameters.

1 48. The storage medium as claimed in claim 41 wherein the DNA
2 thermodynamic parameters include terminal mismatch parameters.

1 49. The storage medium as claimed in claim 41 wherein the
2 thermodynamic parameters include RNA thermodynamic parameters.

1 50. The storage medium as claimed in claim 41 wherein the
2 thermodynamic parameters include hybrid DNA/RNA thermodynamic parameters.

1 51. The storage medium as claimed in claim 41 wherein the
2 thermodynamic parameters include DNA loop thermodynamic parameters.

1 52. The storage medium as claimed in claim 41 wherein the
2 hybridization information represents top and bottom strand sequences which form
3 a duplex and wherein the hybridization thermodynamics are calculated for the
4 duplex.

1 53. The storage medium as claimed in claim 41 wherein the
2 hybridization information represents at least a section of a target and a length of at
3 least one primer or probe complimentary to the target.

1 54. The storage medium as claimed in claim 53 wherein the
2 hybridization thermodynamics are calculated for a plurality of primers or probes
3 complimentary to the target.

1 55. The storage medium as claimed in claim 41 wherein the
2 hybridization information represents at least a section of a target and a primer or
3 probe.

1 56. The storage medium as claimed in claim 55 wherein a length
2 of the target is longer than a length of the primer or probe and wherein the
3 hybridization thermodynamics are calculated for a best target/primer or target/probe
4 complex and for competitive mismatch complexes.

1 57. The storage medium as claimed in claim 54 wherein
2 hybridization information represents at least a section of a target and a primer or
3 probe and wherein a length of a target is longer than the length of the primer or
4 probe and wherein the hybridization thermodynamics are calculated for a best
5 target/primer or target/probe complex and for competitive target/primer or
6 target/probe complexes.

1 58. The storage medium as claimed in claim 42 wherein the
2 program further executes the step of calculating concentration of each species in a
3 solution at a plurality of temperatures.

1 59. The storage medium as claimed in claim 58 wherein
2 hybridization information also represents a primer or probe and wherein the length
3 of the target is longer than a length of the primer or probe and wherein the
4 hybridization thermodynamics are calculated for a best target/primer or target/probe
5 complex and for competitive mismatch complexes and wherein the program

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6 executes the step of calculating concentration of every species in a solution at a
7 plurality of temperatures.

1 60. The storage medium as claimed in claim 59 wherein the
2 hybridization thermodynamics are calculated for at least two best target/primer or
3 target/probe complexes and for their corresponding competitive mismatch
4 complexes and wherein the program executes the step of correcting for any
5 interactions between the at least two best target/primer or target/probe complexes
6 and their components.

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